Molecular features and toxicological properties of four common pesticides, acetamiprid, deltamethrin, chlorpyriphos and fipronil

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Résumé en anglais	Structural features and selected physicochemical properties of four common pesticides: acetamiprid (neonicotinoid), chlorpyriphos (organophosphate insecticide), deltamethrin (pyrethroid) and fipronil (phenylpyrazole) have been investigated by Density Functional Theory quantum chemical calculations. The high flexible character of these insecticides is revealed by the numerous conformers obtained, located within a 20 kJ mol−1 range in the gas phase. In line with this trend, a redistribution of the energetic minima is observed in water medium. Molecular electrostatic potential calculations provide a ranking of the potential interaction sites of the four insecticides. The theoretical studies reported in the present work are completed by comparative toxicological assays against three aphid strains. Thus, the same toxicity order for the two susceptible strains Myzus persicae 4106A and Acyrthosiphon pisum LSR1: acetamiprid > fipronil > deltamethrin > chlorpyriphos is revealed. In the resistant strain M. persicae 1300145, the toxicity order is modified: acetamiprid > fipronil > chlorpyriphos > deltamethrin. Interestingly, the strain 1300145 which is known to be resistant to neonicotinoids, is also less sensitive to deltamethrin, chlorpyriphos and fipronil.
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